

Chemistry and Materials Science Directorate News

chemistry & materials science CMS

January 2003
Volume 1, No. 1

Featured Articles:

***Biosecurity
and Nanoscience
Laboratory**

***Interview with
David Eaglesham**



**Looking forward
to a great year with
a dynamic team...**

I am excited about our CMS Newsletter and look forward to its quarterly release. Our goal is to provide a brief snapshot of what is happening in CMS—with a focus on science, our program contributions, our facilities, safety and security, new hires,

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Providing scientific excellence and leadership that meets and anticipates the needs of the Laboratory's programs.

A corner on science... from our BioSecurity and NanoScience Laboratory

The BSNL's focus is to develop innovative techniques aimed at preventing or deterring biological and chemical threats. The Laboratory is exploring new applications in analytical science at the molecular scale, discovering how to rapidly identify, image, and detect pathogens in new and innovative ways to enhance U.S. security.

A team of LLNL scientists is working on a way to inhibit and block highly toxic proteins (tetanus and botulinum toxins) that attack the central nervous system and spinal cord of human and animal hosts, causing spastic paralysis and often death. These toxins, indigenous to our natural environment, are used in the medical field, have been ingested by dairy cattle and wildfowl, and are of great interest to terrorist groups or other nations



Loreen Zeller in the Analytical & Nuclear Chemistry Division is one of the co-authors

as a biological weapon. Computational methods, Fourier transform mass spectrometry, and NMR spectroscopy have been useful in identifying novel small molecules that can be used for this purpose.

Published in: *American Chemical Society*, October 2002, 15(10), <http://pubs.acs.org/CRT>

An interview with David Eaglesham...

*"The Laboratory has a unique
opportunity to be the nexus of
U.S. R&D for national security"*

David's decision to move to Livermore was an emotional one due to September 11, 2001. "I watched 9-11 from the top of our street, about 20 miles from the World Trade Center. That certainly influenced my decision to pursue a security mission." David

joined the Laboratory this past October as Chief Technologist for our Directorate. Livermore offers David the Homeland Security mission and work with sensors and detectors. His initial focus will be on developing and coordinating nanoscience and nanotechnology applications for national security. David researched employment at other national laboratories (Sandia, OakRidge, and Brookhaven), but chose Livermore because of its R&D environment and its close proximity to Silicon

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"Interview" *continued from page 1*

Valley. "Livermore is at the intersection of national security, the defense industry and Silicon Valley—a tremendous opportunity." He feels the talent and skills in cutting-edge technology at LLNL can now achieve a broad impact. "In Homeland Security, every US citizen is a potential customer, and the spin-off applications will be in everyday household items."

David is excited about our opportunity to interface between electronics and biology—between materials, biology and chemistry. David's goal is to use his expertise in electronics and photonics technology and apply that to chemical, biological, and radiochemical sensors and detectors to meet the growing needs of the future.



At Bell Labs/Agere Systems, David's most recent position was Product Line Director of Transponders and High-Speed Physical Layers, and previous to that he was the Vice President of Electronic Device Research. While at Bell Labs, he was Director of Semiconductor Research. David has a tremendous record of scientific accomplishment, and extensive experience in manufacturing, setting strategic directions and building synergy between cutting-edge R&D and technology applications. He has a PhD in Physics from Bristol University, Bristol, United Kingdom. Welcome, David!

"Looking Forward" *continued from page 1*

postdoctorate updates, directorate awards and achievements, and news about our staff. In the future, I also intend to use this column to communicate my thinking and views on important issues that affect our life as a directorate.

I am proud to be a part of a dynamic team and look forward to a very exciting, but challenging 2003. The Laboratory and CMS are at a cross roads. We are evolving into a new era, new ways of doing business, and a new frontier—Homeland Security—a term that will likely become an integral part of who and what we are. CMS plays a key role in this new environment and offers tremendous opportunity for all of us to support a very important goal for our nation and to be a part of history that will echo our achievements in the future. At the same time, we have to deliver on our important commitments to the Laboratory programs in stockpile stewardship, the NIF, Energy and Environment and Biology and Biotechnology. It is our tradition of excellence in meeting the demands of the Laboratory and in anticipating its future needs through innovation in science and technology that positions us to be an essential part of anticipating and meeting the challenges and opportunities of the future. We are poised for collective success.

A happy holiday season, and a prosperous New Year to you all!

Cheers, Tomas

What's Happening with B155's Construction and B151's Seismic Upgrade



Building 155, our new 22,000 ft² office facility, is on schedule for occupancy beginning in April 2003. Building 151's seismic upgrade will begin in January 2003 to bring the 1960's-era facility up to current earthquake standards.

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"Construction" *continued from page 2*

For residents of B151 you can expect the drilling and noise to be quite disruptive. We are working to minimize the noise and inconvenience to you in several ways, including adding exterior lighting, limiting drilling during working hours, providing temporary office spaces, and issuing noise-reducing headphones.

Please contact Barbara Pulliam (3-4680), CMS' Program Project Manager for the ISF Line Item, in B151 R1118, if you have any questions about the ISF project or its impact on your work.

We are sorry for the short-term inconvenience, but value your long-term safety...thanks for your patience.

Congratulations to those leaving the Postdoc Program and remaining at LLNL:

ANCD: Carola Laue

CChED: Mitch Anthamatten, Kurt Glaesmann, Brandon Weeks, Louisa Hope-Weeks, and Kevin Vandersall

MSTD: Sonia Letant and Chad Talley

Brian Wirth, former Postdoc Program Director, has left the Laboratory for a faculty position in the Nuclear Engineering Department at the University of California, Berkeley as an Assistant Professor. Congratulations and Best Wishes. We hope to see you often at the Lab!

Safety and Security

A reminder to continue to be vigilant in our work practices relative to handling classified and sensitive information—we must continue to appropriately protect our security assets! Re-read your emails to ensure sensitive information is not contained in the text.

CMS has an excellent overall safety record. Nevertheless, each year several of

you suffer injuries due to slips, trips, and falls. Besides being painful, these accidents can be serious enough to result in lost work days that impact the jobs you do here, as well as the jobs we all have at home. Remember to be cautious on our wet streets. On the brighter side, the days will be getting longer and spring flowers will be glorious, due to such a wet winter!

Tom Arsenlis, new Director of the Postdoc Program...

"I am proud and honored to inherit a program that is serving as the flagship postdoctoral program for other directorates at the Laboratory."



"I was attracted to the Laboratory because of its unique combination of world-class researchers and computational facilities."

Starting in January, Tom's goal will be to strengthen the research profile of the Directorate with the introduction of the H. C. Graboske, Jr. fellowship, to aid in the professional and career development of our postdoctoral researchers, to foster a sense of community among the postdocs in CMS, and to ensure they have a positive experience at the Laboratory.

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News about our Postdocs...

Our Postdoctorate Program just completed its Fall 2002 offsite luncheon at Wente Vineyards on Monday, December 16, 2002. Keynote speaker at the luncheon was Dr. Laurel Haak, Editor of the Postdoc Network at *Science Magazine's* Next Wave.

Recent seminars at our monthly BrownBag series (last Thursday of the month) include:

Nov 21: Dr. Karl Van Bibber, "Nuts and bolts about LDRD proposals"

Oct 31: A conversation with Dr. Edward Teller

Sept 26: Dr Ken Moody, "Radiochemistry, the Stockpile, and National Security"

Postdocs—coming or going?

Please welcome our new Postdocs:

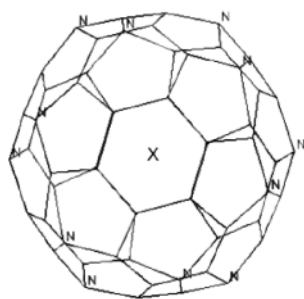
ANCD: Keith Coffee and Bahrad Sokhansanj

CChED: Will Kuo

MSTD: Masato Hiratani, Taira Okita, Christophe Bostedt, and Tim Ratto.

Notable PUBS...

What's in a molecule?



Front view of the S_6 symmetry $C_{48}N_{12}$ structure showing the positioning of all nitrogen atoms. Seven all-carbon hexagons are clearly visible, while the eighth is superimposed on the central ring. X indicates the C_6 symmetry axis through the plane of the paper.

When new materials are discovered it is very important to understand their ground-state properties such as the way in which they are stabilized. Experienced chemists can make a reasonable guess at the mechanism for stability of a new molecule based on "rules of thumb", and often do. For complex systems, however, there is much more to learn from careful modeling.

Recently chemists synthesized an onion-structured, nitrogen-substituted fullerene material. Researchers proposed that the structure of its core "soccer ball," $C_{48}N_{12}$, contains evenly spaced nitrogen atoms, one in each pentagon. Such a distribution would stabilize the molecule by minimizing repulsive nitrogen-nitrogen interactions. But a new theoretical study from CMS chemist M. Riad Manaa has

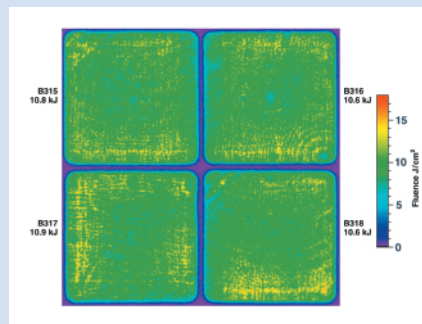
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Did you know?

CMS staff members provided strong support to the recent Defense and Nuclear Technology Director's Review Committee of W Program. Close integration of CMS work into the W effort was evident. Several important presentations and posters were provided on work in support of the W80 Life Extension Program as well as Stockpile Surveillance and Evaluation. The review committee comments were extremely supportive of our work.

CMS staff, as part of the NIF team, made very strong contributions to an important milestone. On Saturday December 21, the NIF B31 bottom quad fired 43 kJ into the RDME calorimeters, completing

the main laser commissioning test plan. This represents a remarkable achievement, making NIF the second most powerful laser in the world even though it is operating at only 1% of its planned final capacity.



NEL 43kJ shot nearfield images

Where were you when the universe was being formed?

Sounds like a question that an intergalactic sergeant Friday might ask of a suspicious asteroid. Well, CMS' geophysical and planetology sleuth, Ian Hutcheon, along with his collaborators Yuri Amelin, Alexander N. Krot, and Alexander A. Ulyanov have helped to answer an important question about the origin of primitive materials and how and when they evolved using isotopic chronometry.

Ian and his team have used a modified secondary ion microprobe or SIMS to identify and trace $^{207}\text{Pb}/^{206}\text{Pb}$ ratios which are used as an isotopic chronometer or cosmic-clock based on radioactive decay of two long-lived radionuclides: ^{235}U and ^{238}U . By precisely determining the age of geological components of two

different chondrites, Acfer 059 and Efremovka to be 4564.7 ± 0.6 and 4567.2 ± 0.6 million years ago respectively, they deduce an interval of 2.5 ± 1.2 million years and have set a limit on the period of formation of chondrite formation. An important result of their work (*Science* 2002 September 6; 297: 1678-1683) <http://www.sciencemag.org/cgi/reprint/297/5587/1678.pdf> is its implications with regards to competing models for chondrite formation, the X-wind, the jet flow and the shock-wave models. In particular, Ian's results suggest that the shock wave model for periods as long as 1 to 3 My is not consistent with the gravitational instability of the protoplanetary disk.

"Postdocs"

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Tom received his PhD from MIT in mechanical engineering with specialization in the continuum mechanics of materials. He joined the Laboratory in February 2001 as a researcher in the Computational Materials Science Group in MSTD. He is interested in the plastic deformation of metals and alloys from microscopic length scales to engineering length scales with a focus of connecting micro-structural evolution of metals to the macroscopic mechanical strength they exhibit.

"Molecule"

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yielded an even more stable structure of $C_{48}N_{12}$ in which the extended aromaticity of eight all-carbon hexagonal rings plays the stabilizing role. See *J. Am. Chem. Soc.*, **124**, 13990 (2002) <http://pubs.acs.org:80/cgi-bin/article.cgi/jacsat/2002/124/i47/pdf/ja0281885.pdf>. Manna and his co-authors, high school student David W. Sprehn, and undergraduate Heather A. Ichord, used density functional theory to show that the top and bottom of the azafullerene each consists of a triphenylene-type unit connected to three nitrogen atoms. The 18 π electrons in each unit are distributed to give the outer rings a benzene-like sextet. The six remaining nitrogen atoms lie around the fullerene's equator.

Newsletter comments:
Contact Dabbie Schleich
schleich1@llnl.gov

Brighter Holidays 2002

The AD, Operations, and Facilities offices sponsored a family from Modesto. The father of this large family had a massive stroke in 1995, leaving him paralyzed and unable to work. Thanks to your generosity and spirit of giving, you have blessed this family of eight for this holiday season.



ANCD sponsored a family of six in the Central Valley—34-year-old parents with four pre-teen to teen daughters sharing a small two-bedroom home. The gifts were generous—someone even knitted gloves for the girls. Thanks to you elves out there!



CChED sponsored the Lopez family from Mexico who live in a small house with barely enough room for their eight members. The father and brother work full time at low paying jobs and are having a difficult time making ends meet.



Thank you Patricia Martinez for being a wonderful Santa to 37 families and delivering gifts to Modesto, Empire, Turlock, Tracy, Patterson, Sacramento, and San Jose. Wow... your reindeer must be exhausted! And thanks to Betty Cuevas, Rosa Yamamoto, Brynn Bollinger, and Beverly Zumwalt for your dedication and support.

For pictures of directorate holiday parties, see our website:
<http://cmsonly.llnl.gov/newnews.html>

CMS Directorate Awards 2002— Celebrating Success!

Allen, Patrick
Bartelt, Maria
Baumann, Ted
Beall, Sharon
Bostedt, Christoph
Brothers, Jenean
Bulatov, Vasily
Campbell, Geoffrey
Coronado, Paul
De Yoreo, James
Elmer, John
Felter, Thomas
Fox, Glenn
Gallagher, Patrick
Gard, Eric
Gash, Alex
Gaylord, Reggie
Genin, Francois
Glaesemann, Kurt
Hackel, Debbie
Hart, Brad
Hrubesh, Larry
Letant, Sonia
Lingenfelter, Allen
McCright, Dan
Orme, Christine
Palmer, Todd

Phinney, Doug
Poco, John
Pulliam, Barbara
Quong, Andrew
Reibold, Bob
Reynolds, John
Satcher, Joe
Schoendienst, Nancy
Simpson, Randy
Sprayberry, Dave
Tillotson, Tom
Virginia Curran
Wong, Joe

Tomas said, "That seven researchers from Livermore were elected this year is a reflection not only of individual talent and achievement, but of the Lab's dynamic research culture. The Lab is a place where I have been able to do cutting-edge science that matters to the Laboratory and the nation, and is recognized by my peers in the broad scientific community."

See the March 2003 issue of *APS News* and <http://www.aps.org> for the Fellowship citation.

Tomas Named Fellow of the American Physical Society

Also see our Awards website and remember...you can nominate someone!

Tomas was elected for his work in computational physics, notably his contributions to multi-scale modeling of materials and seminal research on defect processes in solids under irradiation or high strain-rate conditions.

New Hires as of October 2002...Welcome!

AD Office	David Eaglesham	PhD	Chemical Physics	Bristol University, Bristol, England
ANCD	Keith Coffee	PhD	Chemistry	UC, Riverside
ANCD	Victoria Dias	BS	Biology, General	Cal State University, Hayward
ANCD	Bahrad Sokhansanj	PhD	Engineering	
			Applied Science	UC, Davis
ANCD	Paul Weiss	PhD	Nuclear Physics	Florida State University
CChED	Valerie Eiden			
CChED	I-Feng Kuo	PhD	Chemistry	UC, Irvine
CChED	Heidi Turner	AA	Biochemistry	Diablo Valley College
MRI	Dawn Brosnan			
MSTD	Sumner Day	MS	Geology	UC, Davis
MSTD	Jackson Go	AA	Machine and	
			Mechanical Design	San Joaquin Delta College
MSTD	William Grant	MS	Chemistry	University of Colorado, Denver
MSTD	Masato Hiratani	PhD	Physics	Michigan Tech University
SAT	Nancy Thomson			
SAT	Holly Werner	LBS	Child Development	Cornell University

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